XOR Computer Interest Group 2004/08/19

X-RAY SERVER

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GM/CA CAT at Advanced Photon Source

What is X-ray Server?

X-ray Server is a public project operational at the APS since 1997 with the goals to explore novel network technologies for providing wide scientific community with access to personal research results, establishing scientific collaborations, and refining scientific software.

The Server provides Web-based access to a number of programs developed by the author in the field of X-ray diffraction and scattering. The software code operates directly on the Server available for use without downloading. Currently seven programs are accessible that have been used more than **90,000** times.

Currently at:

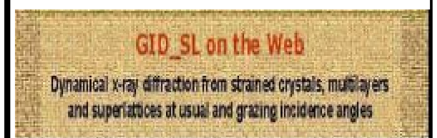
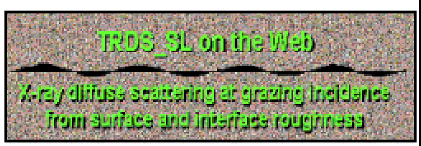
http://sergey.gmca.aps.anl.gov

Before was at:

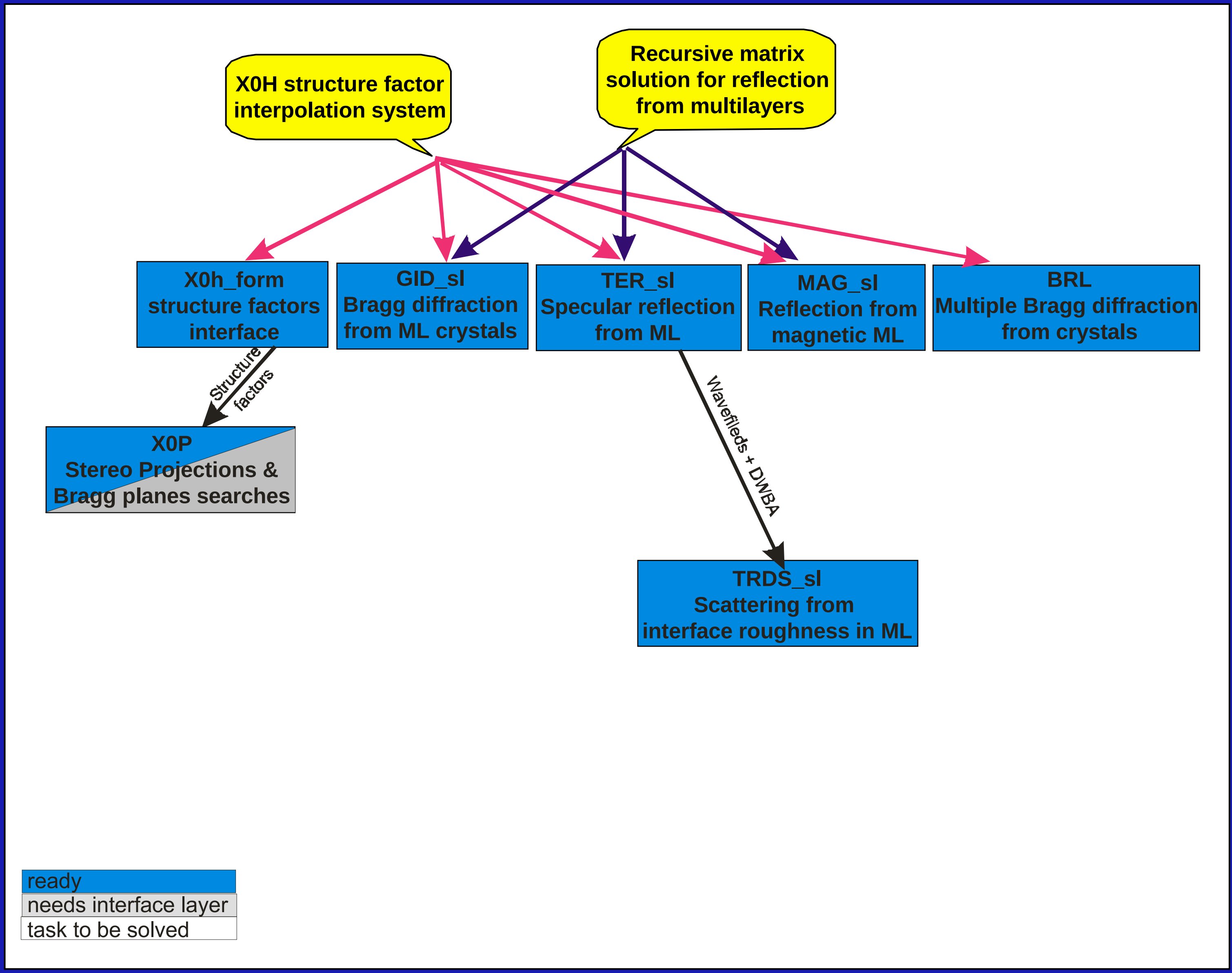
http://sergey.bio.aps.anl.gov

Software available through X-ray Server

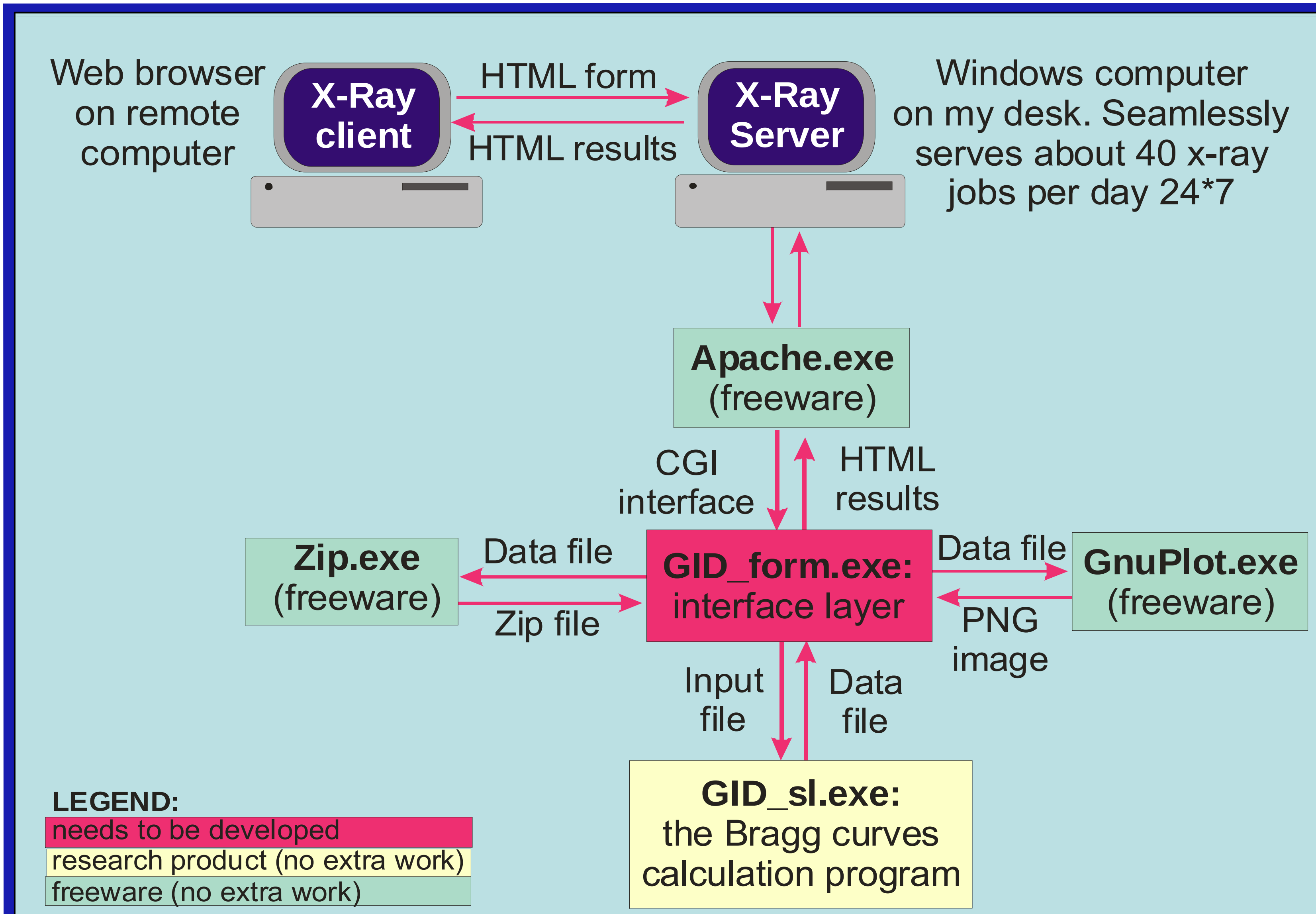
This site has been online since 1997 and has served 90194 x-ray jobs

	***X0h*** **interpolates dielectric susceptibilities x_0 and x_h for some crystals and other materials in wide range of x-ray wavelengths with the option to compare data from different databases.** ***X0h-search*** **is a tool to search for Bragg planes under various conditions.**	**42597** jobs
	***GID_SL on the Web*** **calculates x-ray diffraction curves of strained crystals and multilayers for any Bragg-case diffraction with scans around arbitrary axis. It replaces Takagi-Taupin equations for extremely asymmetric and grazing incidence diffraction.**	**22268** jobs
	***TER_SL on the Web*** **calculates x-ray specular reflection from multilayers with interface roughness and transition layers. It uses a new recursive algorithm converging faster than the recursions by Parratt.**	**9387** jobs
	***MAG_SL on the Web*** **calculates x-ray resonant specular reflection from magnetic multilayers with interface roughness and transition layers. It can also supply wavefields for calculations of diffuse scattering from magnetic roughness.**	**8143** jobs
	***TRDS_SL on the Web*** **calculates x-ray diffuse scattering from interface roughness. It implements several different models of roughness and can simulate effects of skew roughness transfer, dependence of interface-interface roughness correlations on lateral size of roughness and x-ray scattering from atomic steps.**	**7228** jobs
	***BRL on the Web*** **applies a novel algorithm to calculate multiple Bragg diffraction of x-rays including the cases of x-ray waves grazing along the crystal surface and Bragg angles at 90 degr.**	**571** jobs

Server structure



How it works


Web browser on remote computer
X-Ray client
HTML form
HTML results
X-Ray Server
Windows computer on my desk. Seamlessly serves about 40 x-ray jobs per day 24*7
Apache.exe (freeware)
CGI interface
HTML results
Zip.exe (freeware)
Data file
Zip file
GID_form.exe: interface layer
Data file
PNG image
GnuPlot.exe (freeware)
Input file
Data file
GID_sl.exe: the Bragg curves calculation program
LEGEND:
needs to be developed
research product (no extra work)
freeware (no extra work)

Background algorithm

X0h calculates material susceptibilities χ_0 and χ_h for x-ray wavelength range by interpolating data tabulated in the International Tables for X-ray Crystallography and several other tables.
The highlight of ***X0h*** is the way it interpolates the dispersion corrections *df'* and *df"* [1]. The dispersion corrections are calculated with the formulae given by Don Cromer [Acta Crystallogr. vol.18 (1965) p.17-23]:

$$df' = \sum_{k=1}^{N_S} g_k P(X_k, N_k)$$

$$df'' = 0.5\pi \sum_{k=1}^{N_S} g_k (N_k - 1) / X_k^{N_k - 1}$$

First, X0h applies the above equations to known tabulated dispersion corrections and evaluates g_k. Then, it uses calculated g_k to find the dispersion corrections of interest.

Once the χ_0 and χ_h are found, ***X0h*** can fulfill a lot of useful service tasks like evaluating the HWFM of Bragg peaks, searching for Bragg reflections that satisfy certain conditions, and *etc*.

[1] O.M.Lugovskaya & S.A.Stepanov, (1991) Sov. Phys. Crystallogr. **36**, 478-471.

X0h on the Web!!!

Web input form

X-rays:

- ○ Wavelength (A):
- ○ Energy (keV):
- ◉ Characteristic line: Cu-Ka1 ?

Target:

- ◉ Crystal: Silicon ?
- ○ Other material: ?
- ○ Chemical formula: and density (g/cm^3):

Reflection:

Miller indices: 1 1 1

Database Options for dispersion corrections df1 , df2:

- ◉ Use X0h data (5-25 keV or 0.5-2.5 A) -- recommended for Bragg diffraction.
- ○ Use Henke data (0.01-30 keV or 0.4-1200 A) -- recommended for soft x-rays.
- ○ Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)
- ○ Compare results for all of the above sources.

Get X0h! Reset

Example web results

Structure :	Silicon
Symmetry :	Cubic
Density (gm/cm^3) :	2.3293
Unit cell constants (A) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
Poisson Ratio :	0.2800
Composition: Element -- N_sites (Sites occupation)	Si -- 8 (1.000)
X-ray line :	Cu-Ka1
Wavelength (A) :	1.54056
Energy (keV) :	8.04778
Closest absorption edge (keV) :	1.84 (for element **Si**)
Database for df$_1$, df$_2$:	*** X0h (International Tables), 5-25 keV ***
x_{r0} , x_{i0} ($n = 1 + x_{r0}/2 + i*x_{i0}/2$) :	-0.15127E-04 , 0.34955E-06
delta , *eta* ($n = 1$ - *delta* - *i*eta*) :	0.75634E-05 , -0.17477E-06
? Absorption factor (1/cm) and length (um) :	142.56 , 70.144
? Extinction length at TER (A) :	63.033
? Critical angle for TER (degr., mrad) :	0.22287 , 3.8898 GET THE CURVE !
Reflection :	(1 1 1)
Bragg angle (degr.) :	14.221
Interplanar spacing (A) :	3.1355
sin(QB) , cos(QB) :	0.24566 , 0.96936
tan(QB) , cotan(QB) :	0.25343 , 3.9459
sin(2*QB) , cos(2*QB) :	0.47627 , 0.87930
Polarization :	***Sigma***
$\|x_{rh}\|$, $\|x_{ih}\|$:	0.79801E-05 , 0.24314E-06
Phase difference (x_{rh} - x_{ih}) :	1.0000 * pi
Relative intensity (x_h / x_0) :	52.765 %
? Symmetric Laue-case extinction length (um) :	18.705
? Symmetric Bragg-case extinction length (um) :	1.5089
? ..... Double-crystal curve FWHM (arcsec., urad) :	9.7797 , 47.413
? ..... Darwin curve FWHM (arcsec., urad) :	6.9153 , 33.526 GET THE CURVE !
Polarization :	***Pi***
$\|x_{rh}\|$, $\|x_{ih}\|$:	0.70169E-05 , 0.21274E-06
Phase difference (x_{rh} - x_{ih}) :	1.0000 * pi
Relative intensity (x_h / x_0) :	46.396 %
? Symmetric Laue-case extinction length (um) :	21.273
? Symmetric Bragg-case extinction length (um) :	1.7160
? ..... Double-crystal curve FWHM (arcsec., urad) :	8.5992 , 41.690
? ..... Darwin curve FWHM (arcsec., urad) :	6.0806 , 29.479 GET THE CURVE !

Web input form and results

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X-rays:

- ○ Wavelength (A): [ ]
- ○ Energy (keV):
- ◉ Characteristic line: Cu-Ka1 ?

Crystal:

Select code: Silicon ?

Bragg planes range:

From: 1 0 0 To: 1 1 1

Bragg angle range:

From: 0. To: 30.

Intensity control:

Minimum |xh/x0| (%): 0.

Database option for dispersion corrections df1, df2:

- ◉ Use X0h data (5-25 keV or 0.5-2.5 A) -- recommended for Bragg diffraction.
- ○ Use Henke data (0.01-30 keV or 0.4-1200 A) -- recommended for soft x-rays.
- ○ Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)

Find only those Bragg planes which make certain angles to the surface:

Surface plane indices: 1 0 0

- ◉ Planes make angles from Theta1 to Theta2
- ○ Planes make angles from Theta1 to (Bragg_Angle - Theta2)
- ○ Planes make angles from (Bragg_Angle - Theta1) to (Bragg_Angle - Theta2)

Theta1: 0. Theta2: 180.

Find Planes! Reset

SEARCH CONDITIONS :

Crystal:	Silicon
Symmetry group:	Cubic
Density (gm/cm^3) :	2.3293
Unit cell constants (A) :	5.4309 , 5.4309 , 5.4309
Unit cell angles (degr.) :	90.000 , 90.000 , 90.000
X-ray wavelength (Angstrom) :	1.540562
X-ray energy (keV) :	8.047777
X-ray characteristic line :	Cu-Ka1
Bragg planes range :	(1 0 0) -- (1 1 1)
Bragg angles range :	0.0000 -- 30.0000
Minimum intensity (xh/x0) :	0.0000%
Surface :	(1 0 0)
Planes angles to surface :	From Theta1 to Theta2
Theta1, Theta2 :	0.0000 -- 180.0000

SEARCH RESULTS :

Planes found: 4. Planes being displayed: 4

hkl	Angle to surface	Bragg angle
(1 0 0)	0.0000	8.1540
(1 0 1)	45.0000	11.5711
(1 1 0)	45.0000	11.5711
(1 1 1)	54.7356	14.2211

GID_SL on the Web

Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

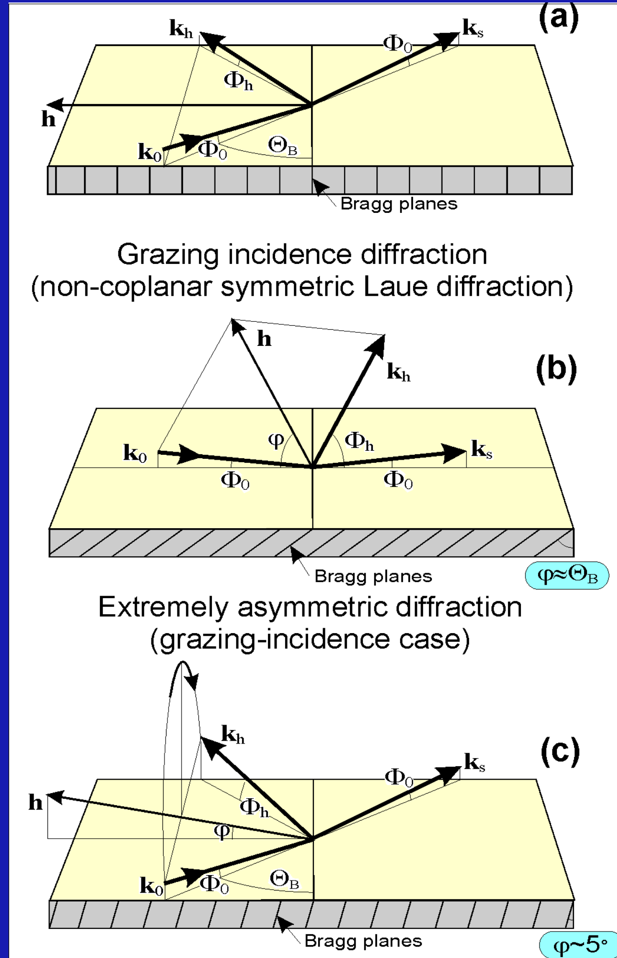
Background algorithm

GID_sl (Grazing Incidence Diffraction from Superlattices) was originally developed for GID (Fig.1a) from multilayers, but then extended to arbitrary Bragg case including coplanar (Fig.1b) and non coplanar asymmetric diffraction (Fig.1c).

The program can calculate Bragg diffraction from imperfect crystals with given profiles of normal lattice strains da(z)/a, dielectric susceptibilities $\chi_0(z)$, $\chi_h(z)$, and interface roughness height σ(z).

The advantage of ***GID_sl*** over most of other Bragg diffraction simulation software is that it takes into account specular reflection and refraction of X-rays at crystal surface and interfaces in multilayers. ***GID_sl*** implements a "discrete" algorithm, i.e. the crystal is subdivided onto "perfect" sublayers and the reflection from the whole stack is calculated with the help of (2x2) recursive matrix algorithm.

Replaces Takagi-Taupin equations for GID!



Grazing incidence diffraction (non-coplanar symmetric Laue diffraction)

Extremely asymmetric diffraction (grazing-incidence case)

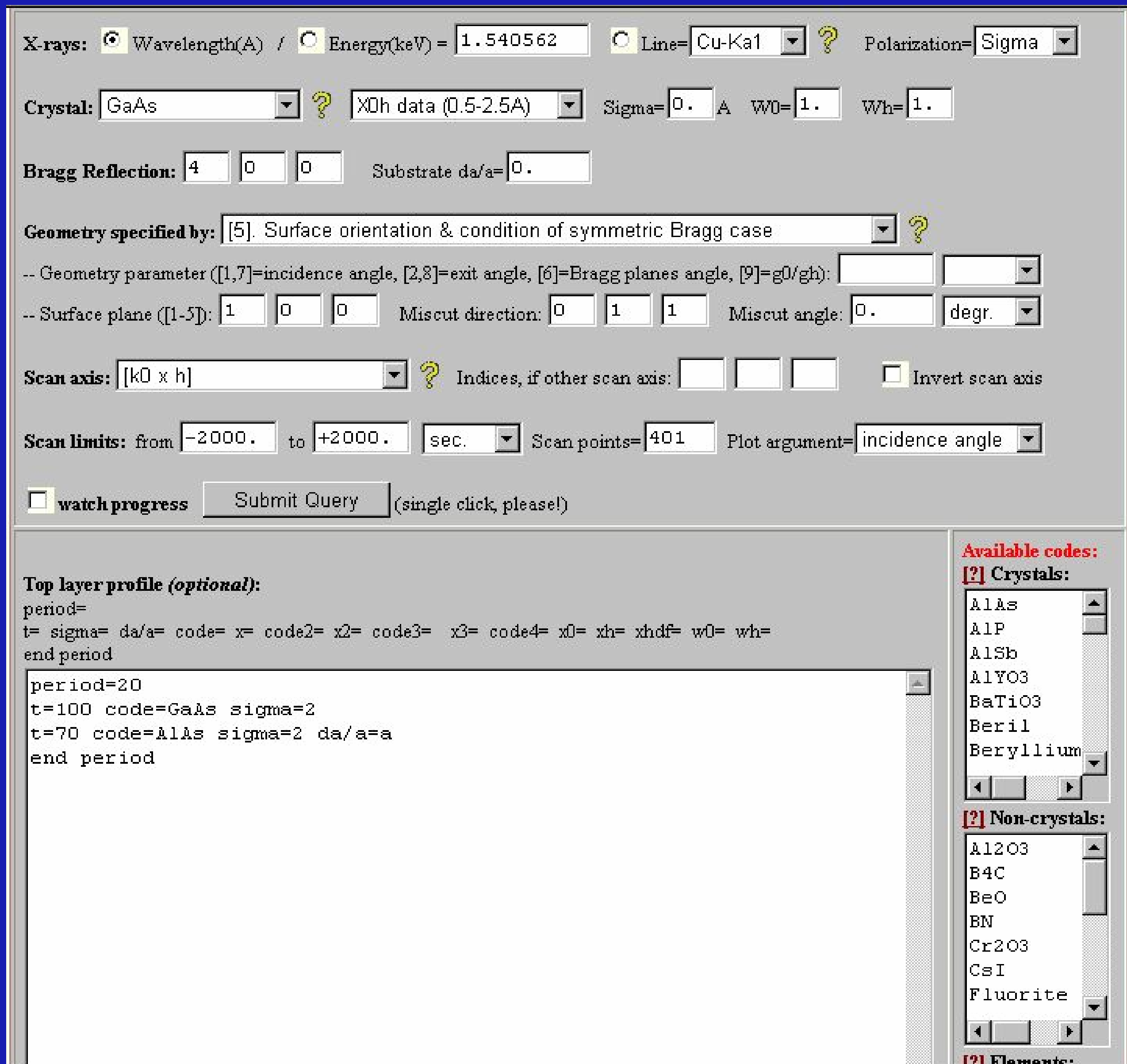
Grazing Bragg-Laue diffraction (non-coplanar asymmetric diffraction)

S.A.Stepanov, E.A.Kondrashkina, R.Koehler, D.V.Novikov, G.Materlik, and S.M.Durbin, Phys. Rev. B, v.**57**, No 8, p. 4829-4841, (1998).

GID_SL on the Web

Dynamical x-ray diffraction from strained crystals, multilayers and superlattices at usual and grazing incidence angles

Web input form


X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line= Cu-Ka1 ? Polarization= Sigma

Crystal: GaAs ? X0h data (0.5-2.5A) Sigma= 0. A W0= 1. Wh= 1.

Bragg Reflection: 4 0 0 Substrate da/a= 0.

Geometry specified by: [5]. Surface orientation & condition of symmetric Bragg case ?

-- Geometry parameter ([1,7]=incidence angle, [2,8]=exit angle, [6]=Bragg planes angle, [9]=g0/gh):

-- Surface plane ([1-5]): 1 0 0 Miscut direction: 0 1 1 Miscut angle: 0. degr.

Scan axis: [k0 x h] ? Indices, if other scan axis: Invert scan axis

Scan limits: from -2000. to +2000. sec. Scan points= 401 Plot argument= incidence angle

watch progress Submit Query (single click, please!)

Top layer profile *(optional)*:
period=
t= sigma= da/a= code= x= code2= x2= code3= x3= code4= x0= xh= xhdf= w0= wh=
end period

```
period=20
t=100 code=GaAs sigma=2
t=70 code=AlAs sigma=2 da/a=a
end period
```

Available codes:
[?] Crystals:
AlAs
AlP
AlSb
AlYO3
BaTiO3
Beril
Beryllium

[?] Non-crystals:
Al2O3
B4C
BeO
BN
Cr2O3
CsI
Fluorite

[?] Elements:

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Example web results

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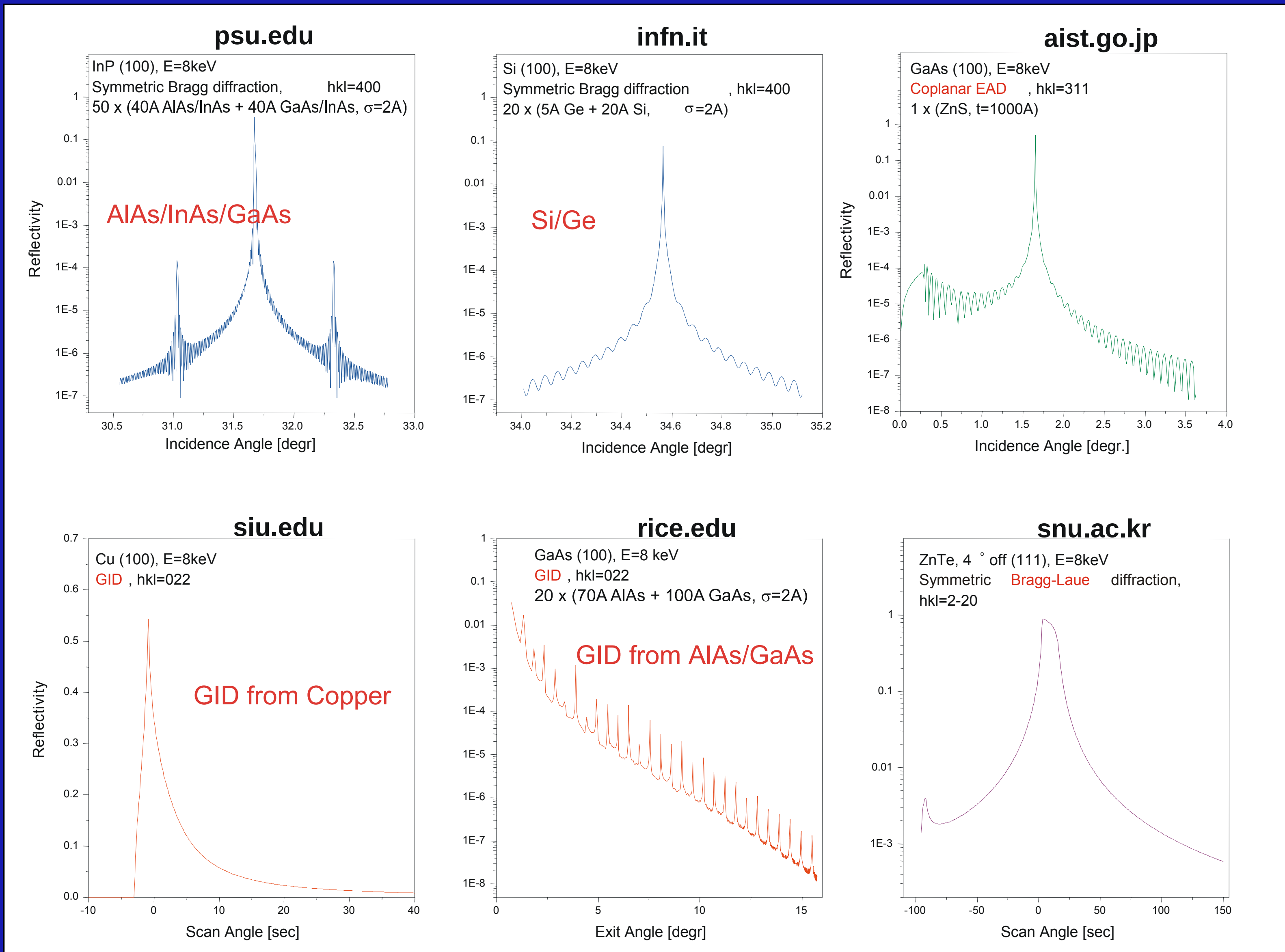


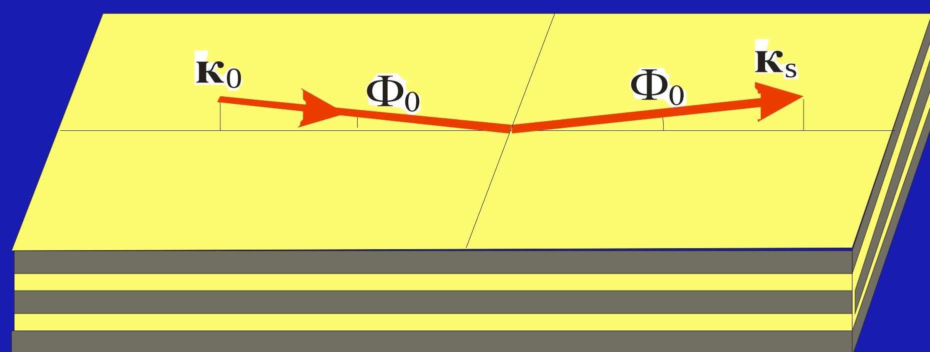
TER_SL on the Web

X-ray specular reflection from multilayers with rough interfaces at grazing incidence

Background model

TER_sl (Total External Reflection) software simulates X-ray specular reflection from multilayers with the account for interface roughness or transition layers.

The advantage of ***TER_sl*** over the well know Parratt recursive technique is a faster convergence of recursions because ***TER_sl*** expresses the reflection from a stack of N layers through the reflectivity of (N-1) layers, while the Parratt technique expresses the reflectivity of N-th layer via that of the underlying (N-1)-th layer.



By-product of ***GID_sl*** -- same recursion algorithm !

S.A.Stepanov, E.A.Kondrashkina, R.Koehler, D.V.Novikov, G.Materlik, and S.M.Durbin, Phys. Rev. B, v.**57**, No 8, p. 4829-4841, (1998).

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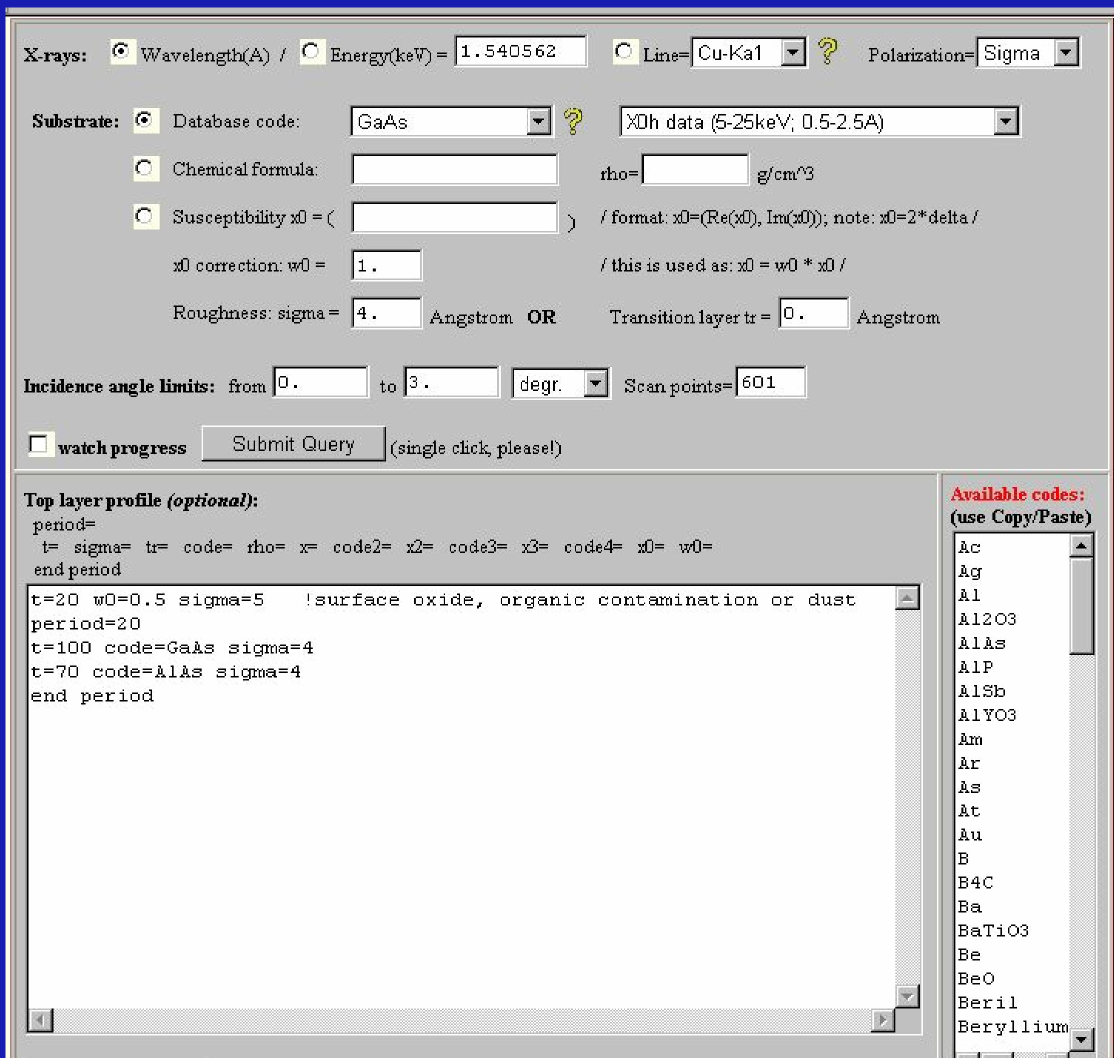
TER_SL on the Web

X-ray specular reflection from multilayers with rough interfaces at grazing incidence

Web form



X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line= Cu-Ka1 ? Polarization= Sigma

Substrate: Database code: GaAs ? X0h data (5-25keV; 0.5-2.5A)

Chemical formula: rho= g/cm^3

Susceptibility x0 = ( ) / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /

x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /

Roughness: sigma = 4. Angstrom **OR** Transition layer tr = 0. Angstrom

Incidence angle limits: from 0. to 3. degr. Scan points= 601

watch progress Submit Query (single click, please!)

Top layer profile *(optional)*:

period=

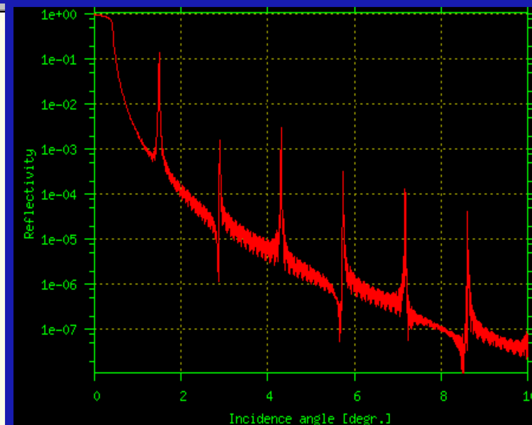
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=

end period

```
t=20 w0=0.5 sigma=5   !surface oxide, organic contamination or dust
period=20
t=100 code=GaAs sigma=4
t=70 code=AlAs sigma=4
end period
```

Available codes:
(use Copy/Paste)

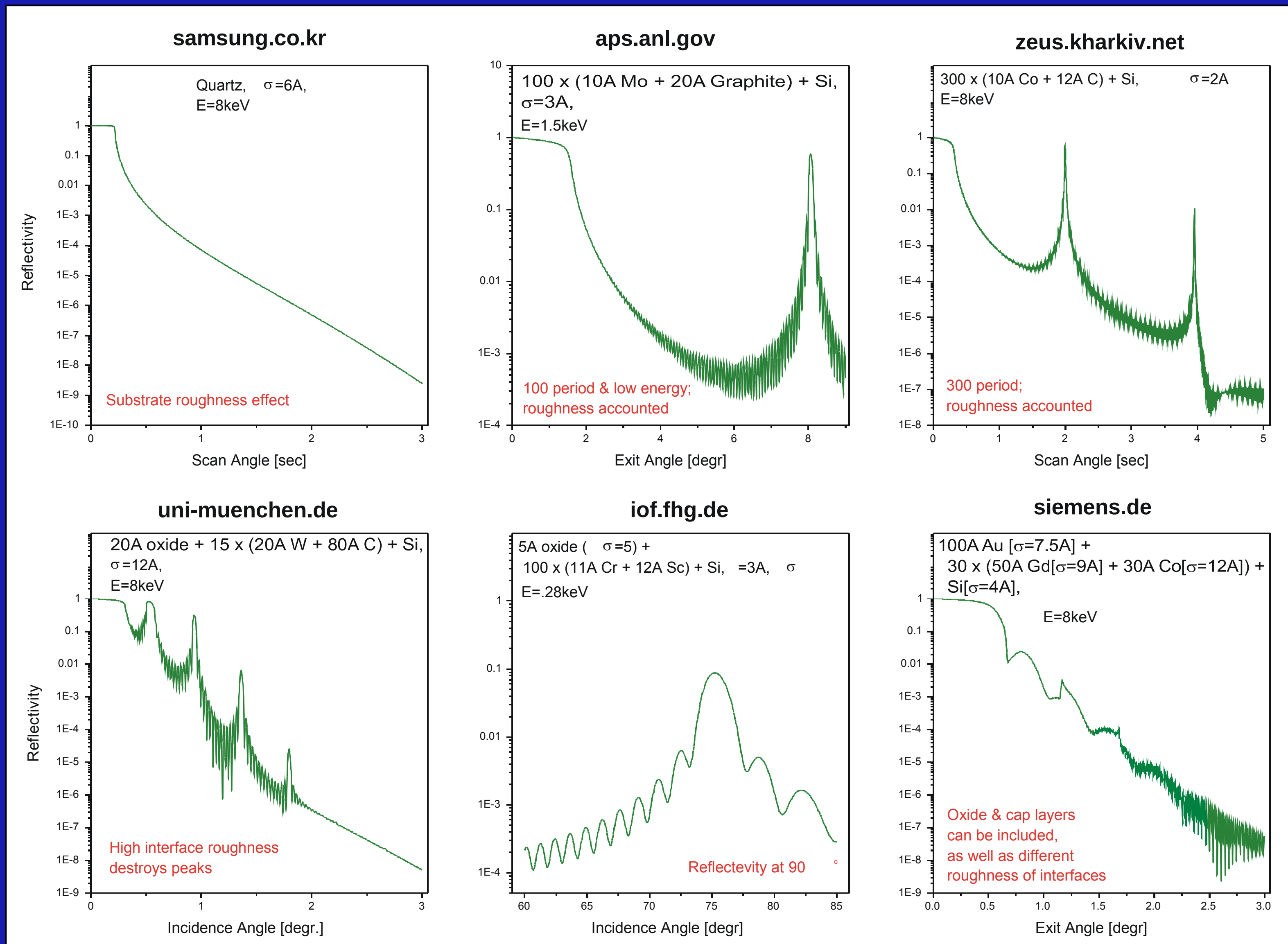
Ac
Ag
Al
Al2O3
AlAs
AlP
AlSb
AlYO3
Am
Ar
As
At
Au
B
B4C
Ba
BaTiO3
Be
BeO
Beril
Beryllium



TER_SL on the Web

X-ray specular reflection from multilayers with rough interfaces at grazing incidence

Example web results



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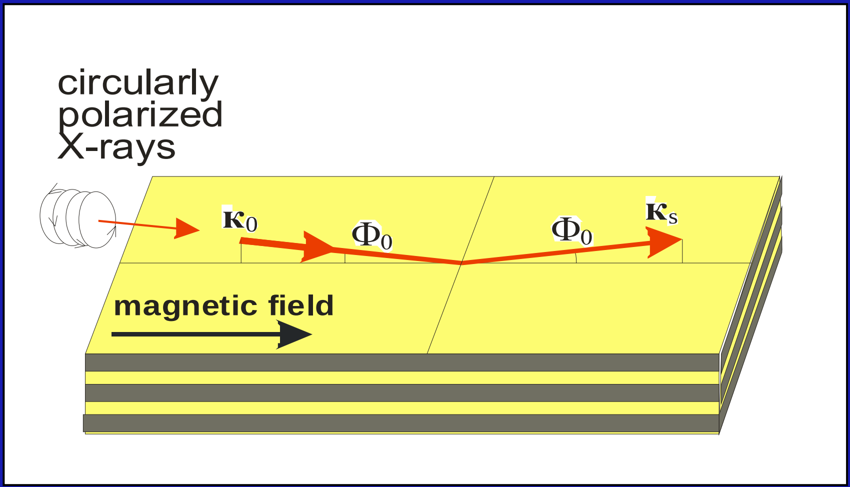
Background algorithm

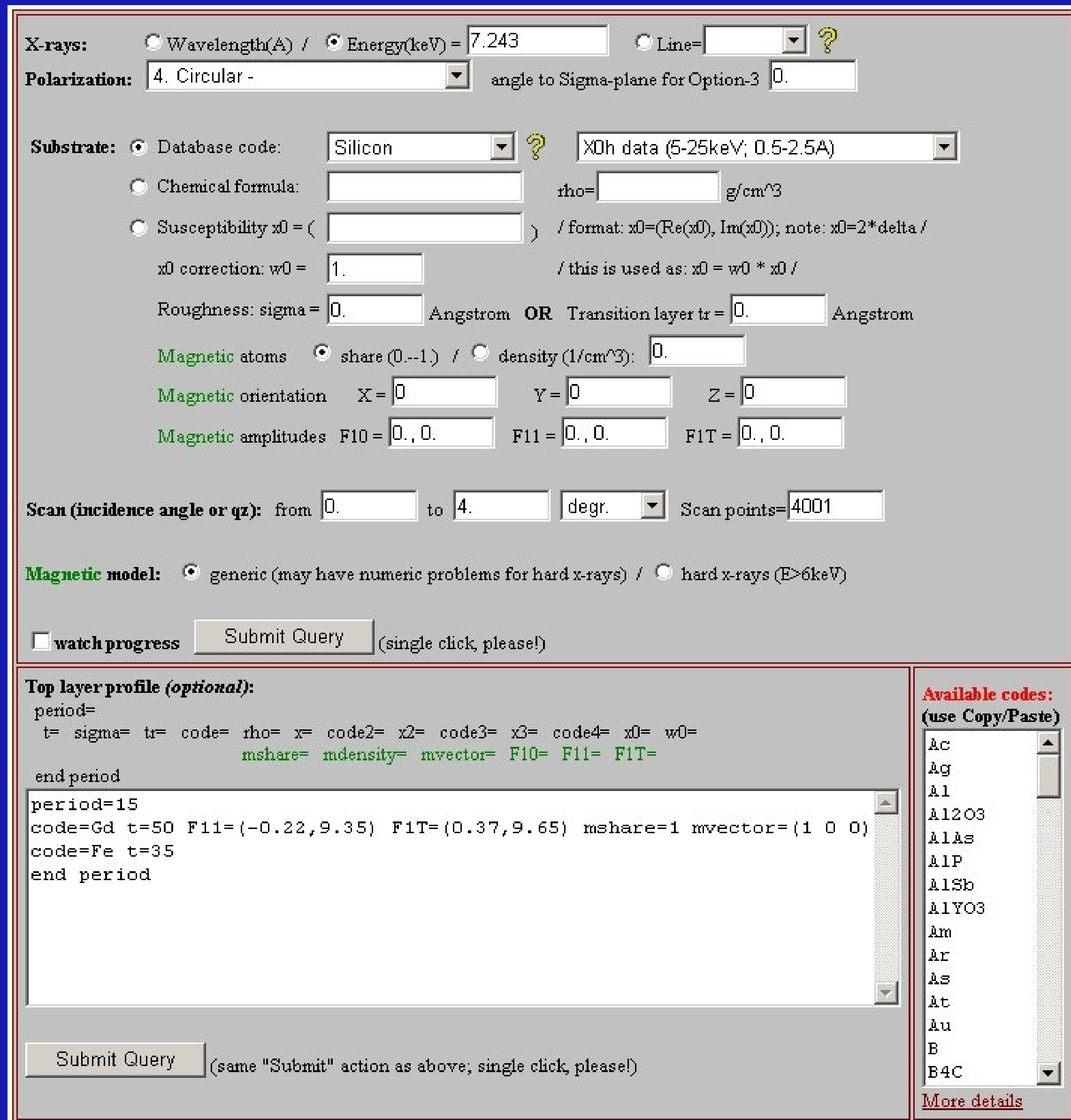
The ***MAG_sl*** program solves the problem of resonant X-ray reflectivity from magnetic multilayers. The major application of X-ray resonant magnetic scattering is to probe thin magnetic films and magnetic multilayers. This is a hot topic related to studying magnetic heads for computer hard drives. However, since in this case the media susceptibility is a tensor, the conventional Parratt technique for calculating X-ray specular reflection is not applicable. The problem is solved in ***MAG_sl*** applying a recursive algorithm for (2x2) scattering matrices similar to that of ***GID_sl***.



S.Stepanov and S.Sinha, Phys. Rev. B, **61** (2000) 15302-15311.

MAG_SL on the Web
X-ray resonant specular reflection from magnetic multilayers

Web form



X-rays: ○ Wavelength(A) / ◉ Energy(keV) = 7.243 ○ Line= ?

Polarization: 4. Circular - angle to Sigma-plane for Option-3 0.

Substrate: ◉ Database code: Silicon ? X0h data (5-25keV; 0.5-2.5A)

○ Chemical formula: rho= g/cm^3

○ Susceptibility x0 = ( ) / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /

x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /

Roughness: sigma = 0. Angstrom **OR** Transition layer tr = 0. Angstrom

Magnetic atoms ◉ share (0.--1.) / ○ density (1/cm^3): 0.

Magnetic orientation X = 0 Y = 0 Z = 0

Magnetic amplitudes F10 = 0., 0. F11 = 0., 0. F1T = 0., 0.

Scan (incidence angle or qz): from 0. to 4. degr. Scan points= 4001

Magnetic model: ◉ generic (may have numeric problems for hard x-rays) / ○ hard x-rays (E>6keV)

☐ **watch progress** Submit Query (single click, please!)

Top layer profile *(optional)*:

period=
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=
mshare= mdensity= mvector= F10= F11= F1T=
end period

```
period=15
code=Gd t=50 F11=(-0.22,9.35) F1T=(0.37,9.65) mshare=1 mvector=(1 0 0)
code=Fe t=35
end period
```

Submit Query (same "Submit" action as above; single click, please!)

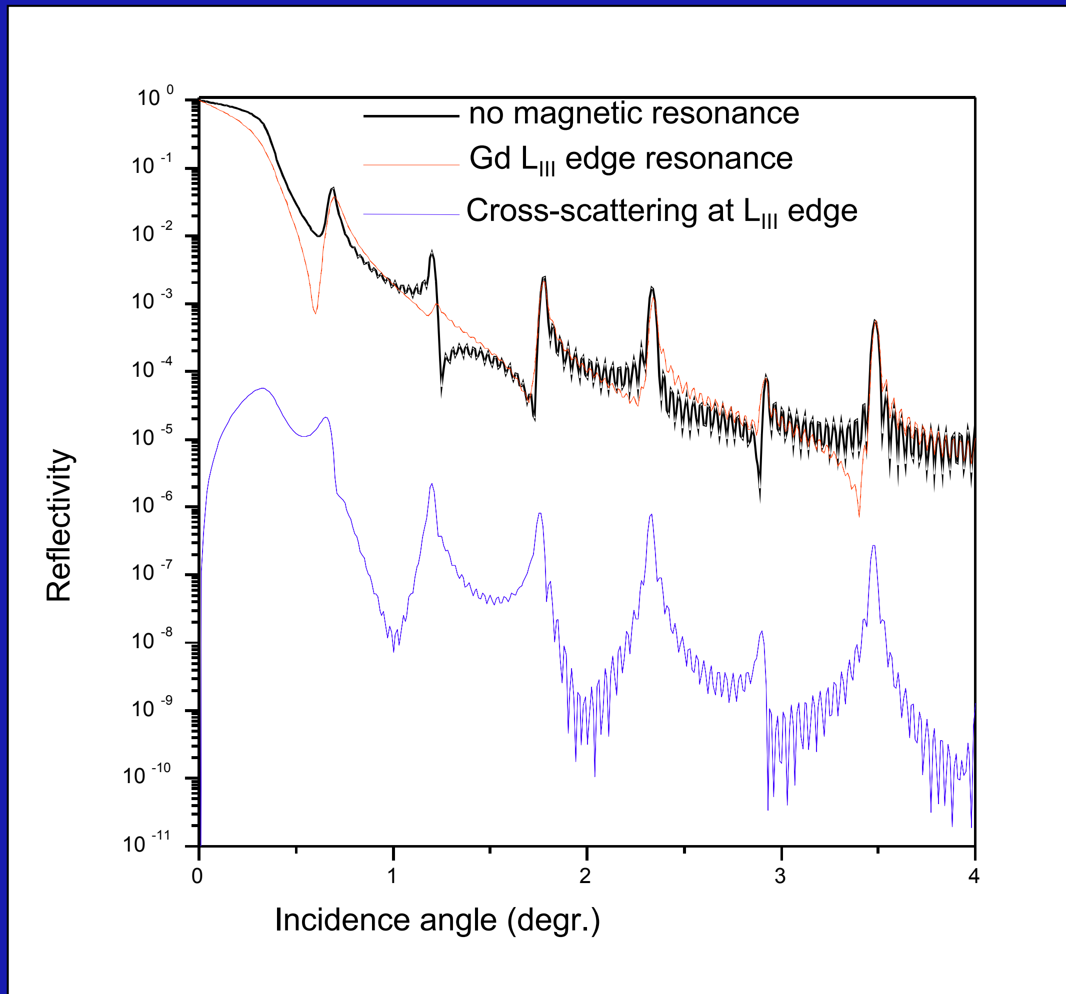
Available codes:
(use Copy/Paste)

Ac
Ag
Al
Al2O3
AlAs
AlP
AlSb
AlYO3
Am
Ar
As
At
Au
B
B4C

More details

MAG_SL on the Web
X-ray resonant specular reflection from magnetic multilayers

Example web results



TRDS_SL on the Web

X-ray diffuse scattering at grazing incidence from surface and interface roughness

Background algorithm - I

TRDS_sl (Total Reflection Diffuse Scattering from Superlatices) was developed for the simulations of X-ray diffuse scattering from interface roughness in multilayers (Fig.1). This program implement a number of different models for interface roughness and for correlations between roughness at different interfaces in multilayers (Fig.2). Notable is the implementation of the model allowing to study wavelength-dependent inheritance of roughness in layer-by-layer grown multilayers (Fig.3).

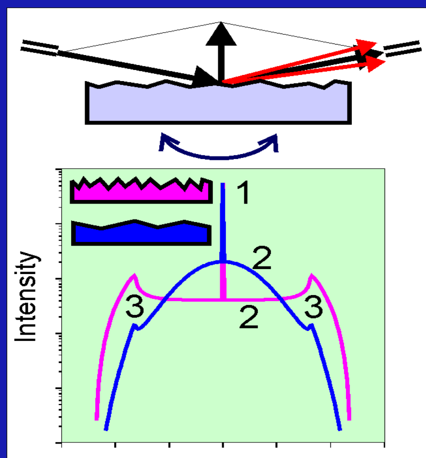


Fig.1. Diffuse scattering of grazing x-rays from surface roughness. 1: specular peak, 2: diffuse scattering for two different lateral scales of roughness, 3: Yoneda peaks at critical angle for total reflection.

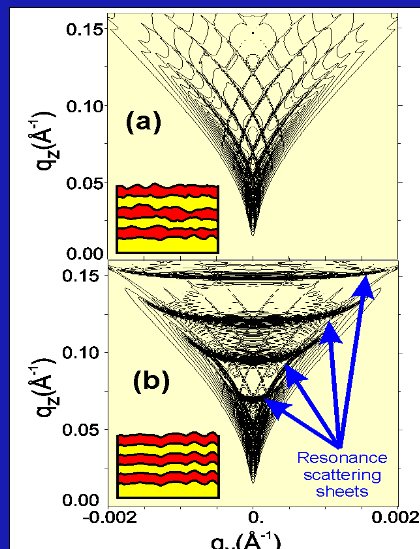


Fig.2. Maps of diffuse scattering from vertically uncorrelated (a) and correlated (b) roughness

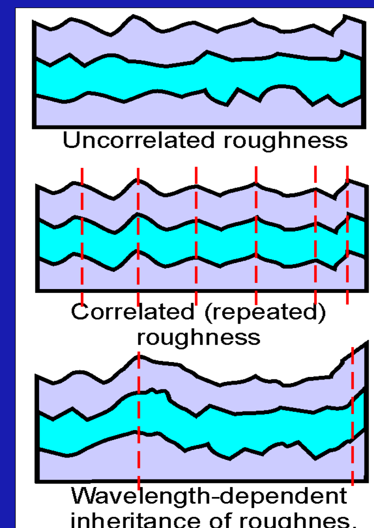


Fig.3. Different models of roughness correlations in multilayers

V.M.Kaganer, S.A.Stepanov & R.Koehler, (1995) Phys. Rev. B **52**, 16369-16372.

TRDS_SL on the Web

X-ray diffuse scattering at grazing incidence from surface and interface roughness

Background algorithm - II

Another notable models implemented in ***TRDS_sl*** are the X-ray scattering from atomic steps on vicinal interfaces and the scattering due to inclined roughness transfer in crystalline multilayers (Fig.4). Both of those effects provide asymmetry of x-ray diffuse scattering (Fig.5), but each of different kind.

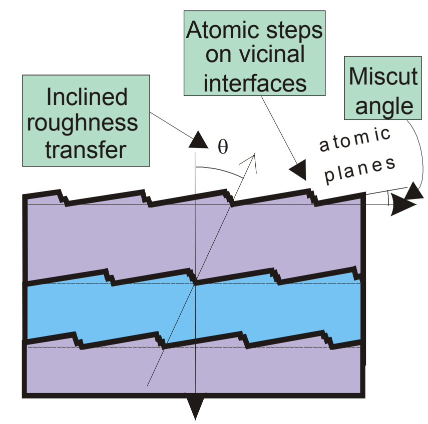


Fig.4. Asymmetric rougness of vicinal interfaces and skew roughness transfer in crystals.

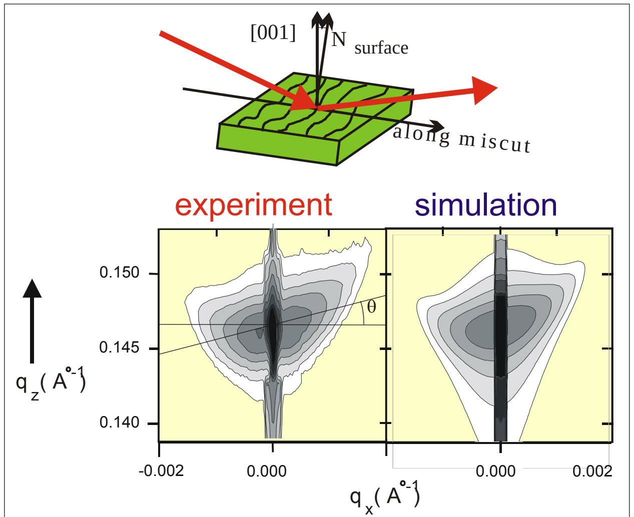


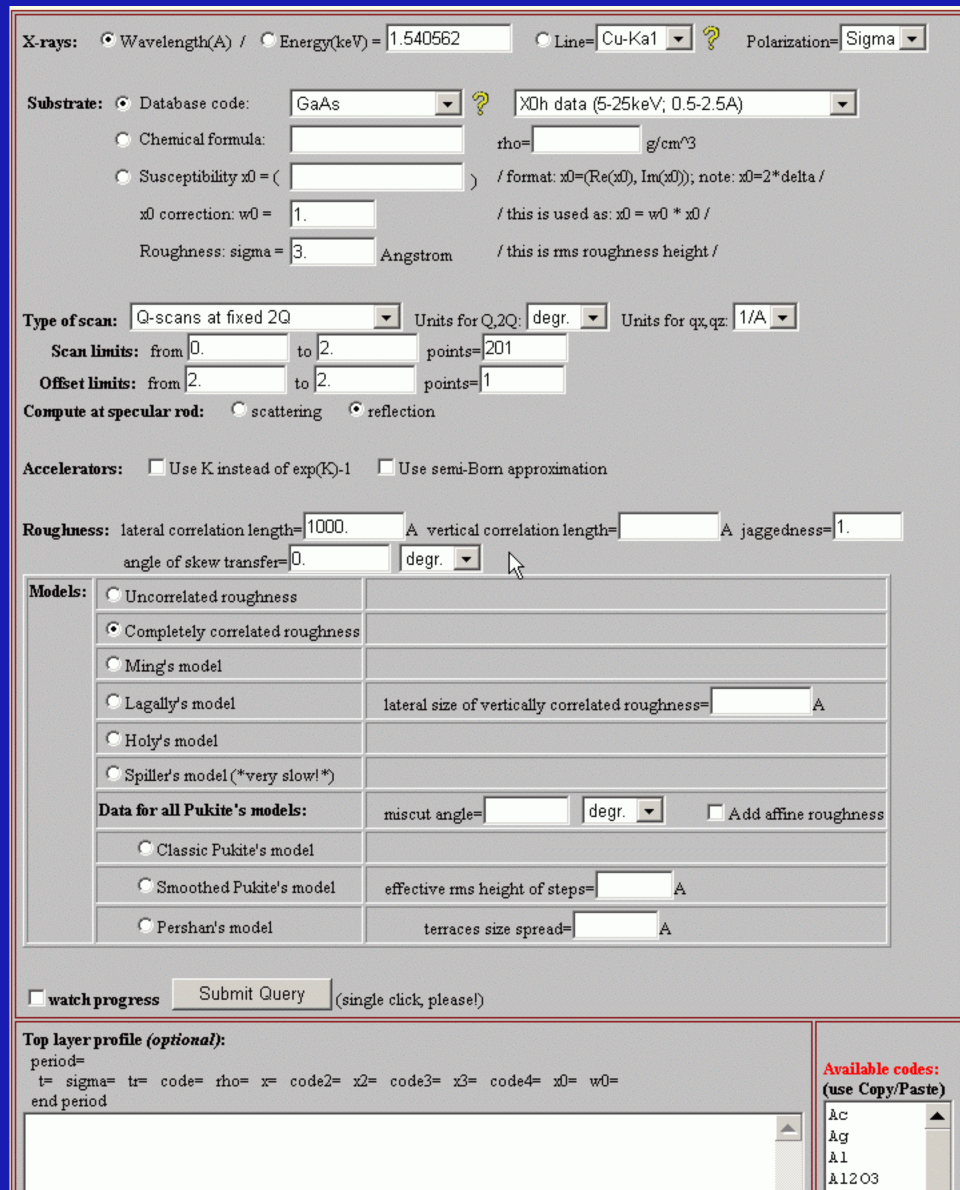
Fig.5. Simulations of inclined roughness transfer in AlAs/GaAs superlattice.

E.A.Kondrashkina, S.A.Stepanov, R.Opitz, M.Schmidbauer, R.Koehler, R.Hey, M.Wassermeier, and D.V.Novikov,

Phys. Rev. B, v.**56**, No 16, p. 10469-10482, (1997).

TRDS_SL on the Web
X-ray diffuse scattering at grazing incidence
from surface and interface roughness

Web form


X-rays: Wavelength(A) / Energy(keV) = 1.540562 Line= Cu-Ka1 ? Polarization= Sigma

Substrate: Database code: GaAs ? X0h data (5-25keV; 0.5-2.5A)
Chemical formula: rho= g/cm^3
Susceptibility x0 = ( ) / format: x0=(Re(x0), Im(x0)); note: x0=2*delta /
x0 correction: w0 = 1. / this is used as: x0 = w0 * x0 /
Roughness: sigma = 3. Angstrom / this is rms roughness height /

Type of scan: Q-scans at fixed 2Q Units for Q,2Q: degr. Units for qx,qz: 1/A
Scan limits: from 0. to 2. points= 201
Offset limits: from 2. to 2. points= 1
Compute at specular rod: scattering reflection

Accelerators: Use K instead of exp(K)-1 Use semi-Born approximation

Roughness: lateral correlation length= 1000. A vertical correlation length= A jaggedness= 1.
angle of skew transfer= 0. degr.

Models:
Uncorrelated roughness
Completely correlated roughness
Ming's model
Lagally's model lateral size of vertically correlated roughness= A
Holy's model
Spiller's model (*very slow!*)
Data for all Pukite's models: miscut angle= degr. Add affine roughness
Classic Pukite's model
Smoothed Pukite's model effective rms height of steps= A
Pershan's model terraces size spread= A

watch progress Submit Query (single click, please!)

Top layer profile *(optional)*:
period=
t= sigma= tr= code= rho= x= code2= x2= code3= x3= code4= x0= w0=
end period

Available codes:
(use Copy/Paste)
Ac
Ag
Al
Al2O3

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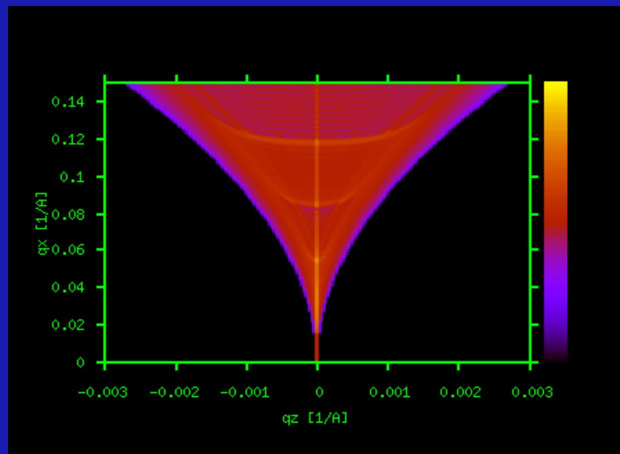
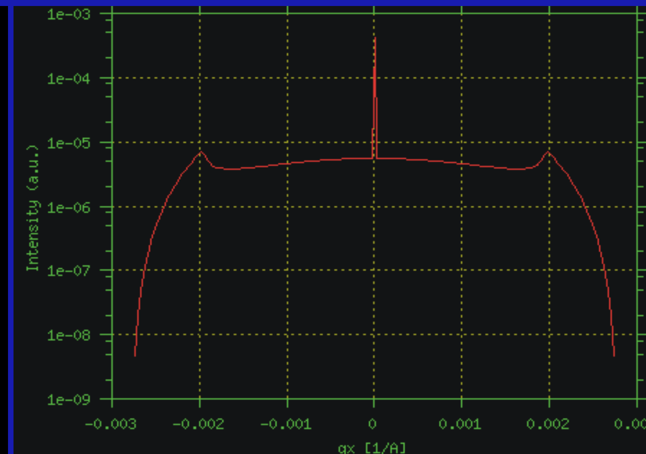
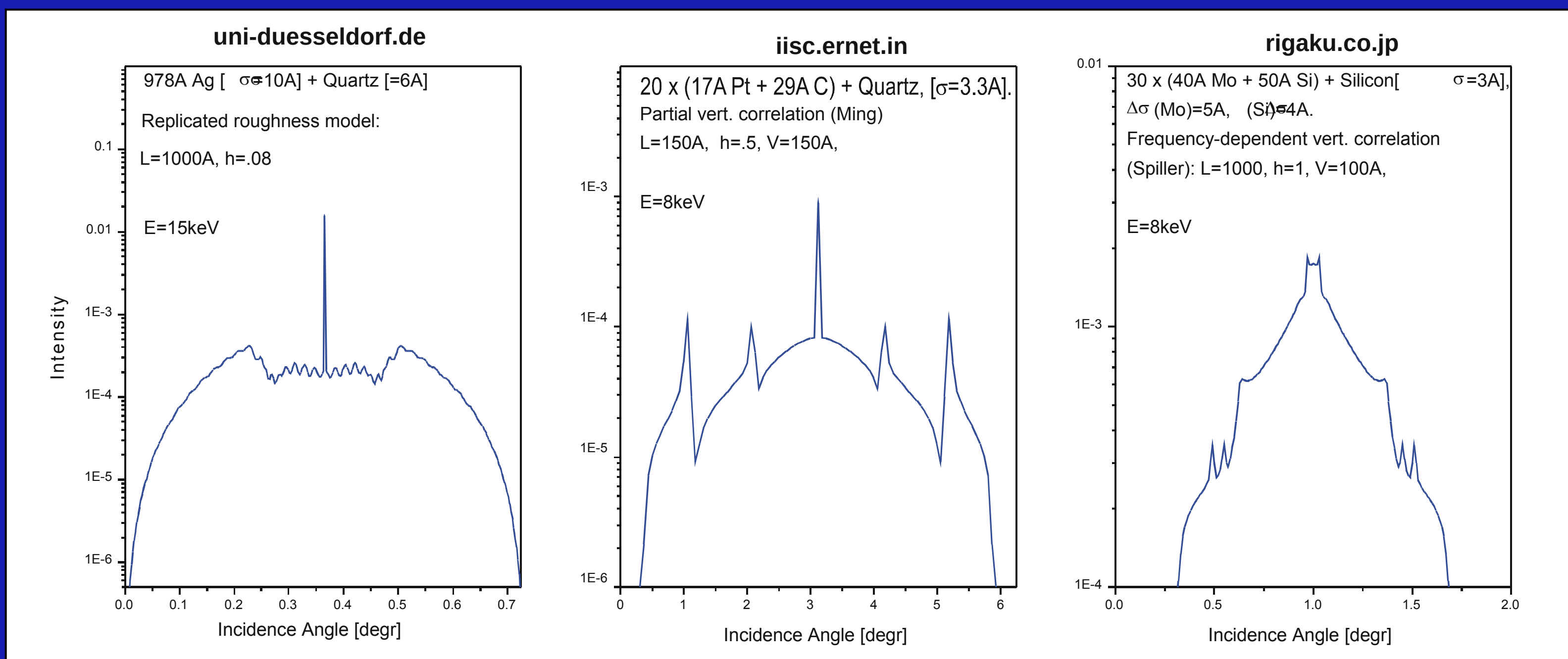
TRDS_SL on the Web

X-ray diffuse scattering at grazing incidence from surface and interface roughness

Example web results





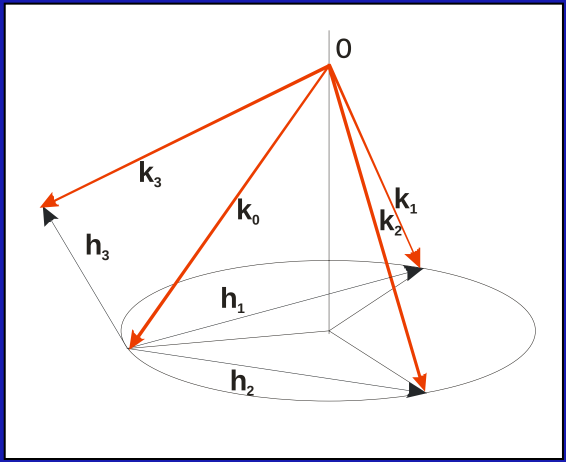


Background algorithm

BRL (Bragg/Laue) calculates multiple Bragg diffraction patterns with the algorithm based on the extended dynamical diffraction theory.

Typically the calculations of multiple Bragg diffraction are reduced to the eigenvalue problem for a 2N*2N scattering matrix. However, when the diffraction geometry involves grazing X-ray waves, the calculations are reduced to the eigenvalue problem for 4N*4N scattering matrix [Colella, Acta Cryst. **A30** (1974) 413].

BRL implements an algorithm where the calculations are reduced to a *generalized* eigenvalue problem for 2(N+Ns)*2(N+Ns) scattering matrix where Ns is the number of grazing waves. Thus, if there are no grazing waves, the matrix size is 2N*2N and if all of the waves are grazing it becomes 4N*4N. In some cases the calculations are reduced dramatically.



S.Stepanov and A.Ulyanenkov, Acta Cryst. **A50** (1994) 579-585.

BRL on the Web
X-ray multiple Bragg/Laue diffraction

Web form

Target:

Crystal:	Silicon			
Surface:	Base plane:	1	1	1
	Miscut direction:	1	-1	0
	Miscut angle:	0.	degr.	

Reflections:

Reflex-1:	1	1	1
Reflex-2:	2	2	0
Index search range:	5		
Min. Intensity filter: (|xh/x0|*100% > ...)	0.1		

X-rays:

- **Wavelength (A):**
- **Energy (keV):**
- **Characteristic line:** Cu-Ka1
- **Fixed by coplanar case**
- **Fixed by Reflex-3:**

Database Options for dispersion corrections df1, df2:

- **Use X0h data (5-25 keV or 0.5-2.5 A) -- *recommended***
- **Use Henke data (0.01-30 keV or 0.4-1200 A)**
- **Use Brennan-Cowan data (0.03-700 keV or 0.02-400 A)**

Submit Reset

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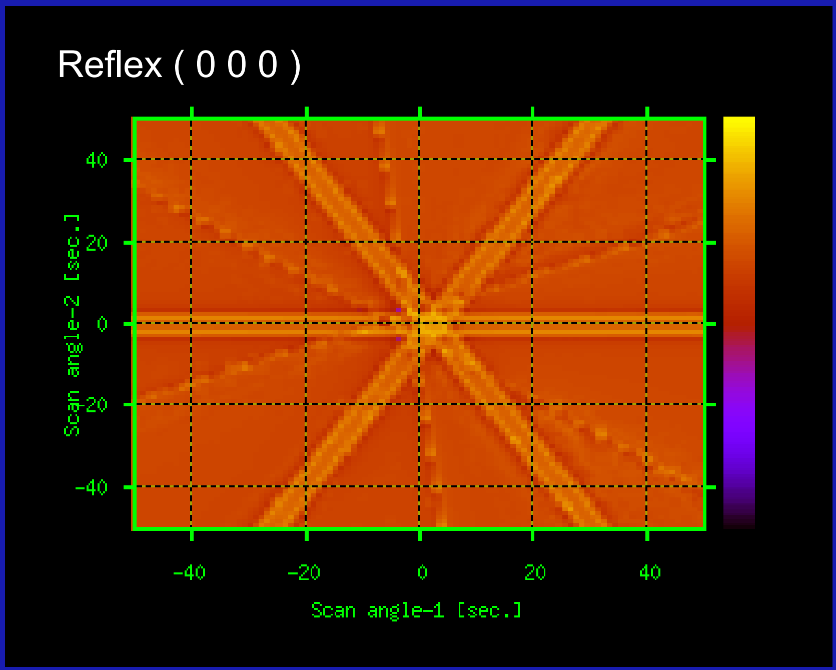
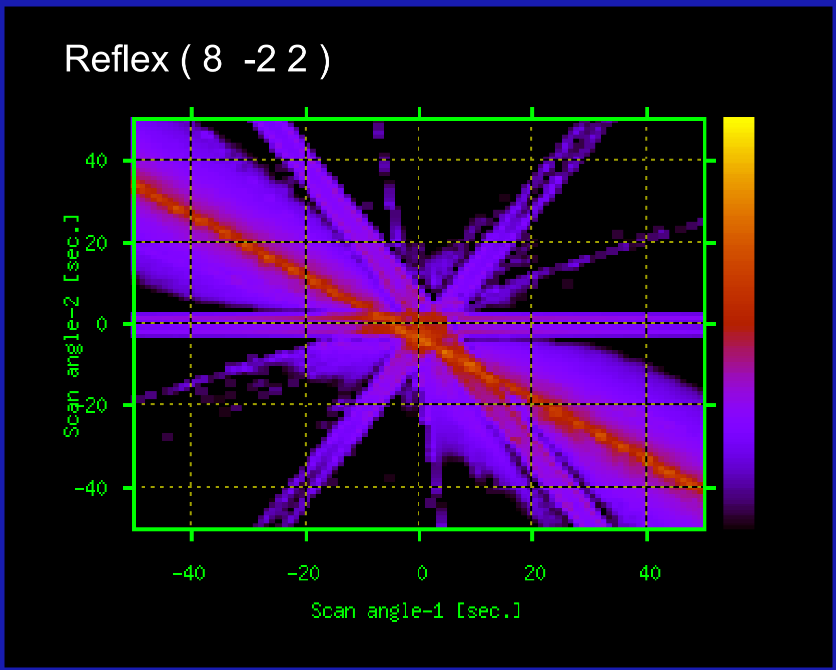
BRL on the Web

X-ray multiple Bragg/Laue diffraction

Example web results

monash.edu.au

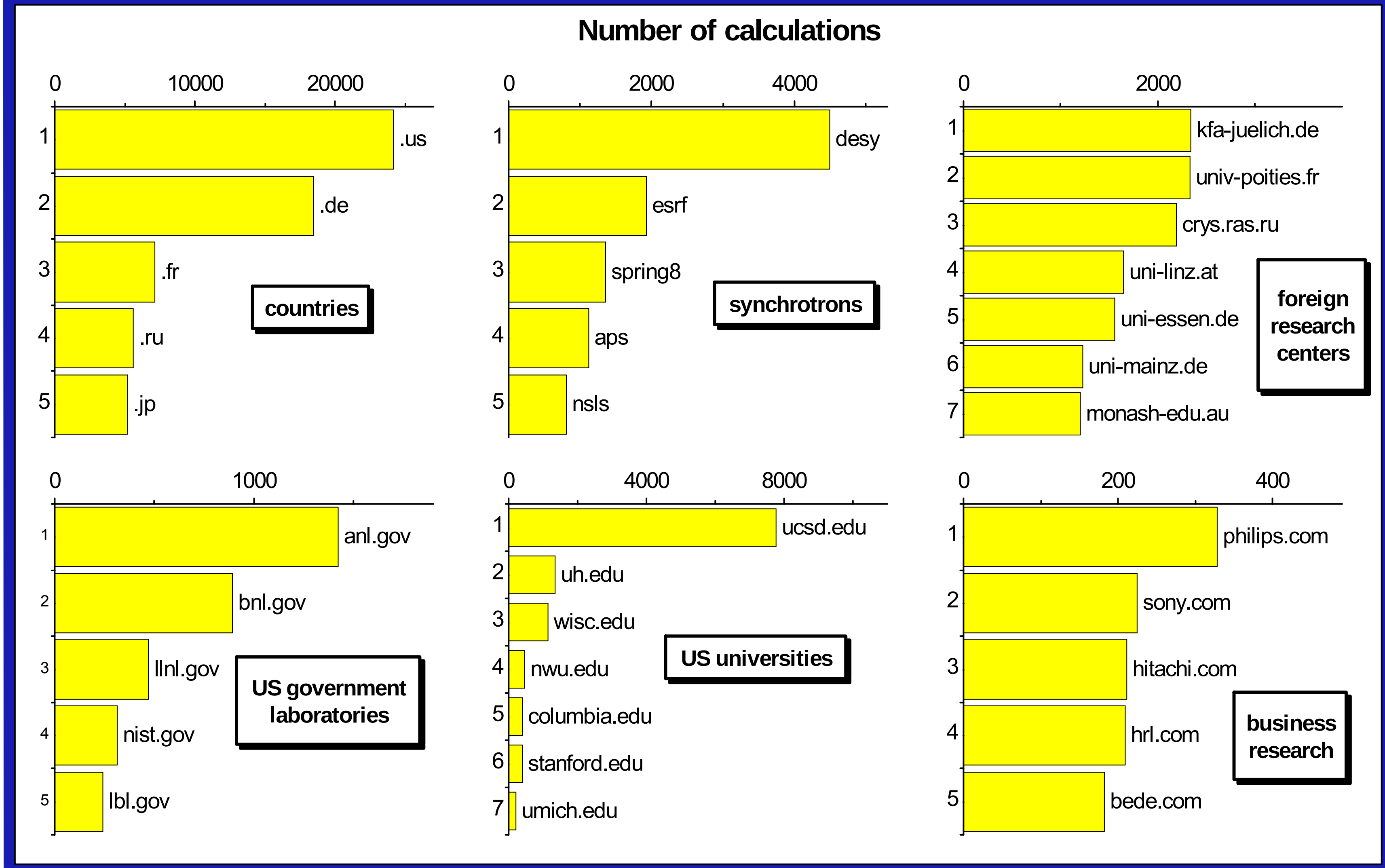




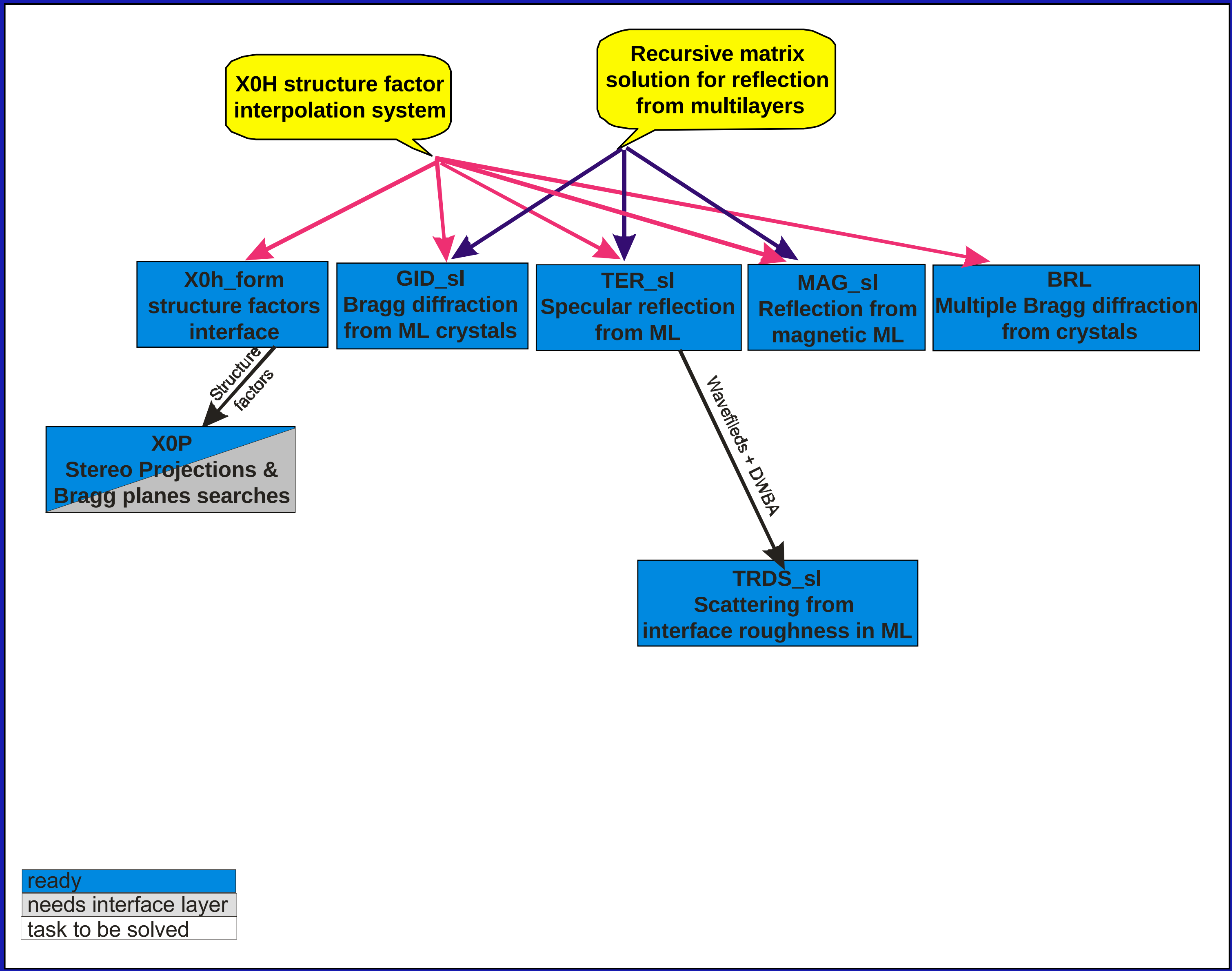
Some maps produced by 10-wave case calculations

(Silicon, λ= 0.6968004107A)

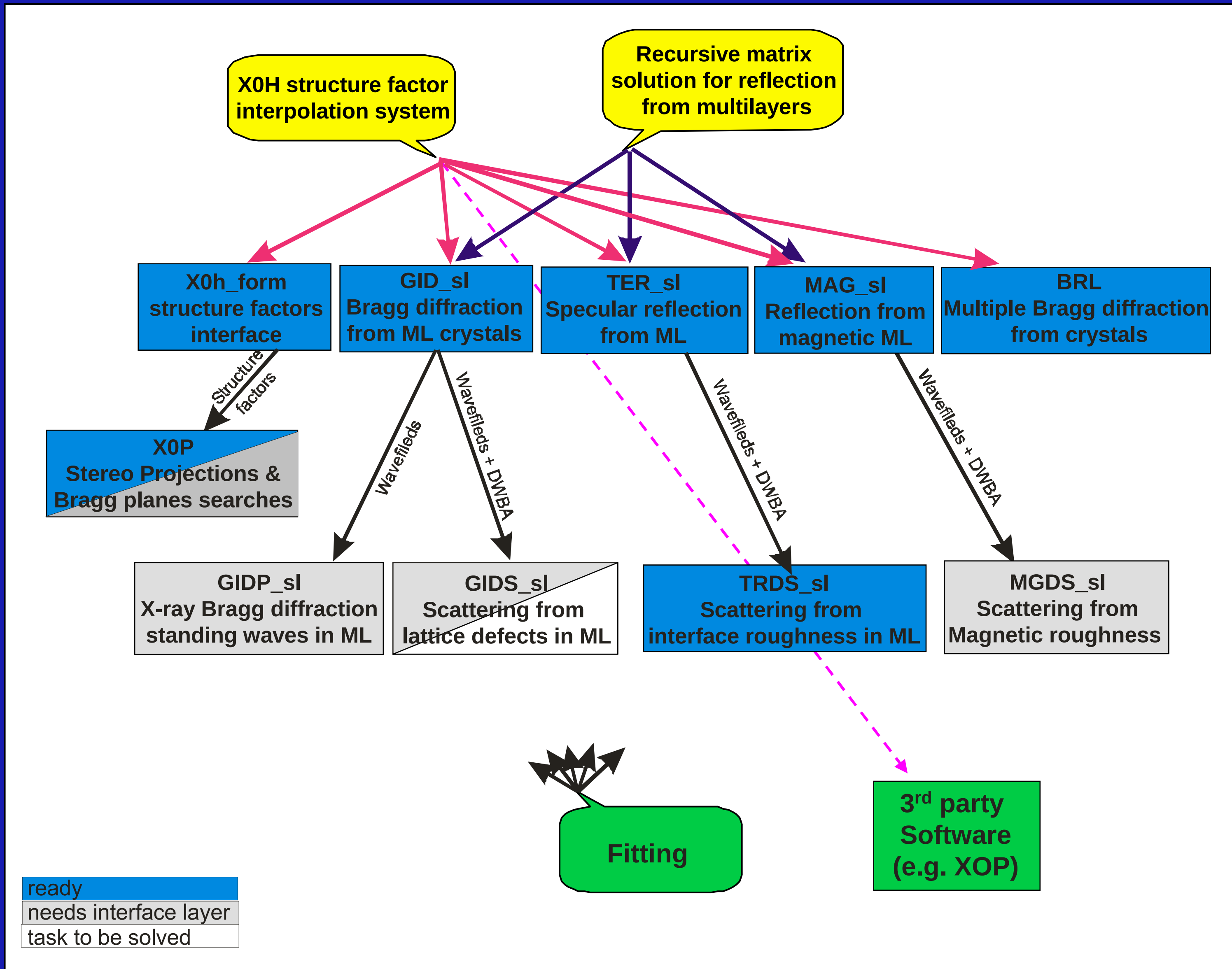
Some X-ray Server statistics



Present server structure



Future Server plans



Conclusions

We have given 7-years test to a new technology of sharing research results. It was proven to be:

- Complimentary to a scientific publication
- Reaching wide audience with small extra effort
- Great for refining scientific software
- Helping to establish new collaborations
- Beneficial for scientific community

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X-ray Server hosts:

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